Electrode processes of relevance for low temperature fuel cells

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A method is introduced for calculating the stability of reaction intermediates of electrochemical processes as a function of bias on the basis of electronic structure calculations. The method is used in combination with detailed density functional theory (DFT) calculations to develop a description of the free energy landscape of the electrochemical electrode processes of relevance to PEM fuel cells. A physical picture is developed of the trends in the electrocatalytic activity of different transition metals for hydrogen oxidation and oxygen reduction. The same picture can be applied to hydrogen evolution, and the efficiency of different transition metals for this reaction is compared to that of enzymes, hydrogenase and nitrogenase, which catalyse the same reaction. The understanding of the enzyme processes open up the possibility of developing new bio-inspired catalysts.